Electronic Supplementary Information for

Synthesis and Characterisation of Bis(β-ketoaminato) Complexes of Cobalt(II)†

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Includes:

- experimental data for X-ray structure determination of **1b** to **6b**
- DFT optimized metrical parameters and thermochemical data for **1c**, **5c**, and **6c**

Contents

Structure Determination of 1b

Data Collection

A orange needle crystal of $C_{32}H_{28}N_2O_2Co$ having approximate dimensions of 0.07 x 0.07 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX diffractometer with graphite monochromated Mo-Kα radiation.

The data were collected at a temperature of -100.0 ± 0.1°C to a maximum 2θ value of 45.0°. Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 20.0 second exposures. The crystal-to-detector distance was 38.85 mm. Due to weak scattering there was little or no useable data beyond a 2θ value of 45° -- the average I/σ(I) between 42° and 45° 2θ was 1.70.

Data Reduction

Of the 16566 reflections that were collected, 3495 were unique (R_{int} = 0.072); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 6.69 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.687 and 0.954, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. All C-H hydrogen atoms were included in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 3495 reflections and 337 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.085$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.109$$

The standard deviation of an observation of unit weight[5] was 1.00. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.31 and –0.25 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

References

(1) SAINT. Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA. (1997-2003).

(2) SADABS. Bruker Nonius area detector scaling and absorption correction - V2.10, Bruker AXS Inc., Madison, Wisconsin, USA (2003).

(3) SIR97 - Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. (1999) J. Appl. Cryst. 32, 115-119.

(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) SHELXTL Version 5.1. Bruker AXS Inc., Madision, Wisconsin, USA. (1997).

Structure Determination of 2b

Data Collection

A red prism crystal of $C_{34}H_{32}N_2O_2Co$ having approximate dimensions of 0.35 x 0.50 x 0.50 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX diffractometer with graphite monochromated Mo-Kα radiation.

The data were collected at a temperature of -100.0 ± 0.1°C to a maximum 2θ value of 56.2°. Data were collected in a series of φ and ω scans in 0.50° oscillations with 5.0 second exposures. The crystal-to-detector distance was 39.12 mm.

Data Reduction

Of the 30714 reflections that were collected, 6835 were unique (R_{int} = 0.036); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 6.34 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.606 and 0.801, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 6835 reflections and 356 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.053$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma w(Fo^2)^2]^{1/2} = 0.092$$

The standard deviation of an observation of unit weight[5] was 1.05. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.29 and –0.42 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and

McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

References

(1) SAINT. Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA. (1997-2003).

(2) SADABS. Bruker Nonius area detector scaling and absorption correction - V2.10, Bruker AXS Inc., Madison, Wisconsin, USA (2003).

(3) SIR97 - Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C. , Guagliardi A., Moliterni A.G.G., Polidori G.,Spagna R. (1999) J. Appl. Cryst. 32, 115-119.

(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) SHELXTL Version 5.1. Bruker AXS Inc., Madision, Wisconsin, USA. (1997).

Structure Determination of 3b

Data Collection

An orange rod crystal of $C_{36}H_{36}N_2O_2Co$ having approximate dimensions of 0.20 x 0.25 x 0.50 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX diffractometer with graphite monochromated Mo-Kα radiation.

The data were collected at a temperature of -100.0 ± 0.1°C to a maximum 2θ value of 55.8°. Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 10.0 second exposures. The crystal-to-detector distance was 38.85 mm.

Data Reduction

Of the 15483 reflections that were collected, 3588 were unique (R_{int} = 0.032); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 6.04 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.698 and 0.886, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. The material resides on a two-fold rotation axis passing through the central Co atom. All non-hydrogen atoms were refined anisotropically. All C-H hydrogen atoms were included in calculated positions but were not refined. The methyl hydrogens on C4 appeared to be disordered and were calculated in two orientations with half-occupancies. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 3588 reflections and 188 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.039$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.079$$

The standard deviation of an observation of unit weight[5] was 1.03. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.48 and –0.30 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

References

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(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

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(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) SHELXTL Version 5.1. Bruker AXS Inc., Madision, Wisconsin, USA. (1997).

Structure Determination of 4b

Data Collection

A red prism crystal of $C_{36}H_{36}N_2O_2Co$ having approximate dimensions of 0.12 x 0.30 x 0.35 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-Kα radiation.

The data were collected at a temperature of -100.0 ± 0.1°C to a maximum 2θ value of 56.3°. Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 5.0 second exposures. The crystal-to-detector distance was 36.00 mm.

Data Reduction

Of the 23369 reflections that were collected, 3586 were unique (R_{int} = 0.044); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 6.18 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.739 and 0.929, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. The material crystallizes with one half-molecule residing on an inversion center. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 3586 reflections and 189 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.047$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.093$$

The standard deviation of an observation of unit weight[5] was 1.04. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.30 and –0.35 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

References

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(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

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(10) SHELXTL Version 5.1. Bruker AXS Inc., Madision, Wisconsin, USA. (1997).

Structure Determination of 5b

Data Collection

An irregular red crystal of $C_{34}H_{26}N_2O_2F_6Co$ having approximate dimensions of 0.15 x 0.20 x 0.45 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-Kα radiation.

The data were collected at a temperature of -100.0 ± 0.1°C to a maximum 2θ value of 56.0°. Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 20.0 second exposures. The crystal-to-detector distance was 36.00 mm.

Data Reduction

Of the 31180 reflections that were collected, 7546 were unique (R_{int} = 0.041); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 6.13 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.679 and 0.912, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. The material crystallizes with disordered fluorines on each of the CF_3 groups. In each case the disorder was modeled in two orientations, with populations for each fragment refining to approximately 50%. Both C17 and C34 have anomalously low U_{eq} values as compared to their neighbours, as an effect of this disorder in the CF_3 groups. The high degree of thermal motion associated with the fluorine atoms results in their unusually large U_{eq} values. All non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were placed in calculated positions and not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 7546 reflections and 464 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.073$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.117$$

The standard deviation of an observation of unit weight[5] was 0.99. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.40 and –0.40 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

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(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

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(10) SHELXTL Version 5.1. Bruker AXS Inc., Madision, Wisconsin, USA. (1997).

Structure Determination of 6b

Data Collection

An irregular red crystal of $C_{34}H_{32}N_2O_4Co$ having approximate dimensions of 0.08 x 0.13 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX II diffractometer with graphite monochromated Mo-Kα radiation.

The data were collected at a temperature of -100.0 ± 0.1°C to a maximum 2θ value of 50.4°. Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 30.0 second exposures. The crystal-to-detector distance was 36.00 mm.

Data Reduction

Of the 19915 reflections that were collected, 5051 were unique (R_{int} = 0.066); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT[1] software package. The linear absorption coefficient, μ, for Mo-Kα radiation is 6.43 cm^{-1}. Data were corrected for absorption effects using the multi-scan technique (SADABS[2]), with minimum and maximum transmission coefficients of 0.508 and 0.950, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[3]. All non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were placed in calculated positions and not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 5051 reflections and 374 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.097$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.165$$

The standard deviation of an observation of unit weight[5] was 1.07. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.58 and –0.49 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and

McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All refinements were performed using the SHELXTL[10] crystallographic software package of Bruker-AXS.

References

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(4) Least Squares function minimized:

$$\Sigma w(F_o^2-F_c^2)^2$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

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DFT Optimization of 1c B3LYP/LANL2DZ

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.130129	2.491735	-2.085634
2	6	0	-2.271895	2.337294	-1.279959
3	1	0	-3.040614	3.095027	-1.385311
4	6	0	-2.543833	1.302096	-0.331579
5	8	0	-0.104423	1.665527	-2.105713
6	7	0	-1.710984	0.274172	-0.091154
7	7	0	1.711063	-0.274102	-0.091452
8	6	0	2.543810	-1.302051	-0.332083
9	6	0	2.271646	-2.337201	-1.280455
10	1	0	3.040318	-3.094962	-1.385969
11	6	0	1.129726	-2.491574	-2.085920
12	8	0	0.104049	-1.665321	-2.105793
13	27	0	-0.000045	0.000087	-1.089608
14	6	0	1.012778	-3.678860	-3.024039
15	1	0	0.871302	-3.319571	-4.051273
16	1	0	1.894134	-4.326390	-2.986562
17	1	0	0.123724	-4.267309	-2.762371
18	6	0	3.875037	-1.405865	0.407493
19	1	0	4.324858	-0.419567	0.560878
20	1	0	3.742113	-1.861635	1.397064
21	1	0	4.573168	-2.030359	-0.157156
22	6	0	-3.874928	1.405754	0.408252
23	1	0	-4.325243	0.419485	0.560438
24	1	0	-3.741672	1.860160	1.398399
25	1	0	-4.572793	2.031314	-0.155535
26	6	0	-1.013415	3.679030	-3.023769
27	1	0	-1.894788	4.326527	-2.986113
28	1	0	-0.124331	4.267512	-2.762276
29	1	0	-0.872131	3.319751	-4.051032
30	6	0	-1.991730	-0.712908	0.919288
31	6	0	-2.182040	-2.058110	0.530155
32	6	0	-1.992161	-0.382505	2.293359
33	6	0	-2.401351	-3.050569	1.502402
34	1	0	-2.149726	-2.309804	-0.526568
35	6	0	-2.208880	-1.379764	3.261067
36	1	0	-1.801646	0.643762	2.597472
37	6	0	-2.419969	-2.717243	2.871250
38	1	0	-2.552878	-4.081692	1.191202
39	1	0	-2.206353	-1.113628	4.315841
40	1	0	-2.587489	-3.486708	3.621051
41	6	0	1.991939	0.712851	0.919063
42	6	0	2.182198	2.058099	0.530055
43	6	0	1.992520	0.382304	2.293100
44	6	0	2.401609	3.050454	1.502382
45	1	0	2.149796	2.309904	-0.526639
46	6	0	2.209339	1.379463	3.260890
47	1	0	1.802058	-0.643998	2.597127
48	6	0	2.420369	2.716986	2.871195

```
   49          1             0        2.553112    4.081608    1.191273
   50          1             0        2.206932    1.113210    4.315634
   51          1             0        2.587958    3.486373    3.621060
 -------------------------------------------------------------------

SCF Done:  E(UB+HF-LYP) =  -1257.78334932     A.U. after    1 cycles
             Convg  =    0.5681D-08             -V/T =  2.0543
             S**2   =   3.7596
 Annihilation of the first spin contaminant:
 S**2 before annihilation     3.7596,   after     3.7500

 Zero-point correction=                           0.414342 (Hartree/Particle)
 Thermal correction to Energy=                    0.441711
 Thermal correction to Enthalpy=                  0.442655
 Thermal correction to Gibbs Free Energy=         0.352620
 Sum of electronic and zero-point Energies=          -1257.369008
 Sum of electronic and thermal Energies=             -1257.341638
 Sum of electronic and thermal Enthalpies=           -1257.340694
 Sum of electronic and thermal Free Energies=        -1257.430729
```

DFT Optimization of 5c B3LYP/LANL2DZ

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.621956	-3.129899	2.208361
2	6	0	-0.934023	-2.311492	3.123422
3	1	0	-1.213605	-2.417858	4.165848
4	6	0	0.084193	-1.349741	2.850339
5	8	0	-1.406196	-3.147372	0.909131
6	7	0	0.577472	-1.116411	1.617546
7	7	0	-0.577479	-1.116426	-1.617539
8	6	0	-0.084204	-1.349774	-2.850332
9	6	0	0.934002	-2.311539	-3.123405
10	1	0	1.213575	-2.417925	-4.165831
11	6	0	1.621933	-3.129936	-2.208335
12	8	0	1.406178	-3.147390	-0.909104
13	27	0	-0.000006	-2.153035	0.000009
14	6	0	2.697227	-4.082636	-2.692886
15	1	0	2.420751	-5.110549	-2.425487
16	1	0	2.850684	-4.021670	-3.774307
17	1	0	3.643018	-3.860684	-2.182230
18	6	0	-0.624905	-0.594769	-4.061542
19	1	0	-1.668644	-0.296848	-3.926562
20	1	0	-0.040090	0.315072	-4.250440
21	1	0	-0.551244	-1.222543	-4.954410
22	6	0	0.624889	-0.594714	4.061538
23	1	0	1.668619	-0.296767	3.926544
24	1	0	0.040052	0.315114	4.250438
25	1	0	0.551254	-1.222485	4.954411
26	6	0	-2.697266	-4.082576	2.692920
27	1	0	-2.850727	-4.021594	3.774340
28	1	0	-3.643052	-3.860616	2.182259
29	1	0	-2.420805	-5.110497	2.425535
30	6	0	1.522395	-0.076592	1.346673
31	6	0	2.749959	-0.413806	0.728570
32	6	0	1.222494	1.286005	1.585225
33	6	0	3.664960	0.586828	0.374882
34	1	0	2.970919	-1.458904	0.533110
35	6	0	2.135321	2.287699	1.229616
36	1	0	0.267310	1.556313	2.025540
37	6	0	3.360558	1.939019	0.627717
38	1	0	4.610924	0.318655	-0.085988
39	1	0	1.898368	3.330349	1.420022
40	6	0	-1.522399	-0.076600	-1.346675
41	6	0	-2.749972	-0.413804	-0.728589
42	6	0	-1.222477	1.285997	-1.585207
43	6	0	-3.664968	0.586838	-0.374906
44	1	0	-2.970946	-1.458901	-0.533139
45	6	0	-2.135297	2.287698	-1.229604
46	1	0	-0.267281	1.556298	-2.025502
47	6	0	-3.360548	1.939026	-0.627726
48	1	0	-4.610940	0.318672	0.085950

49	1	0	-1.898328	3.330347	-1.419997
50	6	0	-4.309014	3.011800	-0.197868
51	6	0	4.309038	3.011775	0.197845
52	9	0	-4.250633	4.154108	-1.013451
53	9	0	-4.055959	3.479701	1.116859
54	9	0	-5.648167	2.590029	-0.189552
55	9	0	4.250542	4.154167	1.013299
56	9	0	4.056113	3.479523	-1.116961
57	9	0	5.648205	2.590038	0.189714

```
SCF Done:  E(UB+HF-LYP) =  -1931.89119724     A.U. after    2 cycles
             Convg  =    0.3638D-08             -V/T =  2.0365
             S**2   =   3.7598
 Annihilation of the first spin contaminant:
 S**2 before annihilation     3.7598,   after     3.7500

 Zero-point correction=                           0.421014 (Hartree/Particle)
 Thermal correction to Energy=                    0.456282
 Thermal correction to Enthalpy=                  0.457227
 Thermal correction to Gibbs Free Energy=         0.344300
 Sum of electronic and zero-point Energies=          -1931.470183
 Sum of electronic and thermal Energies=             -1931.434915
 Sum of electronic and thermal Enthalpies=           -1931.433971
 Sum of electronic and thermal Free Energies=        -1931.546898
```

DFT Optimization of 6c B3LYP/LANL2DZ

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.602076	-2.564256	2.232878
2	6	0	-0.915198	-1.729043	3.130187
3	1	0	-1.201249	-1.806345	4.173612
4	6	0	0.119757	-0.784887	2.836878
5	8	0	-1.385504	-2.617985	0.933990
6	7	0	0.613197	-0.581694	1.603757
7	7	0	-0.613189	-0.581709	-1.603748
8	6	0	-0.119751	-0.784923	-2.836866
9	6	0	0.915193	-1.729094	-3.130164
10	1	0	1.201241	-1.806415	-4.173588
11	6	0	1.602064	-2.564301	-2.232844
12	8	0	1.385492	-2.618011	-0.933955
13	27	0	-0.000001	-1.605690	0.000011
14	6	0	2.683297	-3.502174	-2.738522
15	1	0	2.410005	-4.537374	-2.496660
16	1	0	2.838312	-3.414680	-3.818367
17	1	0	3.627142	-3.288328	-2.220482
18	6	0	-0.669704	-0.006571	-4.029247
19	1	0	-1.740065	0.193235	-3.918429
20	1	0	-0.164582	0.962652	-4.133229
21	1	0	-0.506394	-0.568203	-4.953673
22	6	0	0.669706	-0.006515	4.029246
23	1	0	1.740049	0.193364	3.918393
24	1	0	0.164522	0.962673	4.133262
25	1	0	0.506466	-0.568171	4.953671
26	6	0	-2.683321	-3.502109	2.738567
27	1	0	-2.838337	-3.414598	3.818411
28	1	0	-3.627163	-3.288260	2.220523
29	1	0	-2.410041	-4.537316	2.496720
30	6	0	1.608211	0.424849	1.334974
31	6	0	2.862598	0.037589	0.823648
32	6	0	1.327764	1.805386	1.477606
33	6	0	3.836715	0.997799	0.490384
34	1	0	3.069666	-1.019924	0.683622
35	6	0	2.288706	2.768021	1.146074
36	1	0	0.347380	2.119322	1.826145
37	6	0	3.550329	2.367925	0.656270
38	1	0	4.795766	0.666713	0.104651
39	1	0	2.082710	3.829201	1.249360
40	6	0	-1.608203	0.424838	-1.334978
41	6	0	-2.862601	0.037584	-0.823675
42	6	0	-1.327745	1.805375	-1.477595
43	6	0	-3.836718	0.997797	-0.490425
44	1	0	-3.069677	-1.019929	-0.683657
45	6	0	-2.288686	2.768014	-1.146075
46	1	0	-0.347351	2.119307	-1.826110
47	6	0	-3.550321	2.367923	-0.656299
48	1	0	-4.795778	0.666715	-0.104710

49	1	0	-2.082681	3.829193	-1.249350
50	8	0	-4.438434	3.407133	-0.357031
51	8	0	4.438442	3.407131	0.356993
52	6	0	-5.754621	3.066678	0.162374
53	1	0	-6.260414	4.022020	0.316798
54	1	0	-6.323001	2.459909	-0.556701
55	1	0	-5.679604	2.529596	1.118519
56	6	0	5.754618	3.066671	-0.162438
57	1	0	6.260414	4.022011	-0.316868
58	1	0	6.323008	2.459896	0.556623
59	1	0	5.679580	2.529594	-1.118584

SCF Done: E(UB+HF-LYP) = -1486.79744524 A.U. after 1 cycles
Convg = 0.2707D-08 -V/T = 2.0464
S**2 = 3.7596
Annihilation of the first spin contaminant:
S**2 before annihilation 3.7596, after 3.7500

Zero-point correction= 0.478157 (Hartree/Particle)
Thermal correction to Energy= 0.511217
Thermal correction to Enthalpy= 0.512161
Thermal correction to Gibbs Free Energy= 0.408035
Sum of electronic and zero-point Energies= -1486.306358
Sum of electronic and thermal Energies= -1486.273298
Sum of electronic and thermal Enthalpies= -1486.272354
Sum of electronic and thermal Free Energies= -1486.376480